

Chlorotrifluoroethylene

79-38-9 | DTXSID3026485

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: -24.5 °C

Global applicability domain: Inside

Local applicability domain index: 5.58e-01

Confidence level: 6.54e-01

Nearest Neighbors from the Training Set

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Chlorotrifluoroethylene

Measured: -27.8

Predicted: -24.5

Image not found

Trifluoroacetyl chloride

Measured: -27.0

Predicted: -18.8

Image not found

Bromotrifluoroethene

Measured: -1.00

Predicted: -1.18

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Ethene, trifluoro-

Measured: -51.0

Predicted: -38.7